



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 04:54 PM UTC

PDB ID : 9GWZ / pdb_00009gwz
Title : Crystal structure of 23ME-00610 Fab
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Deposited on : 2024-09-27
Resolution : 2.12 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

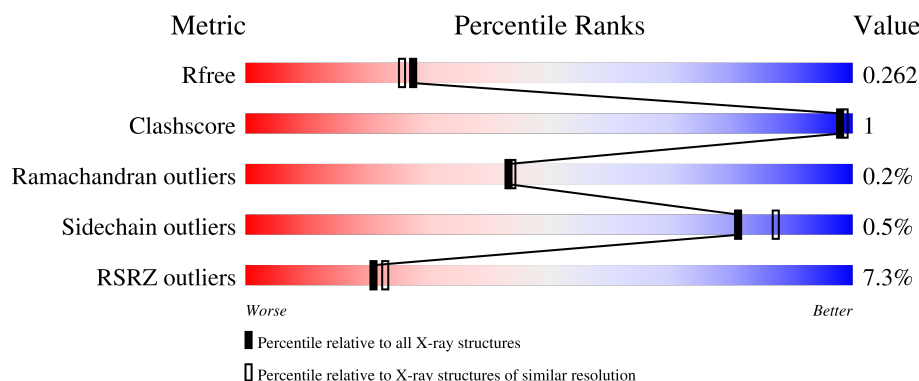
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



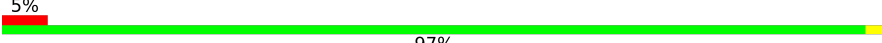
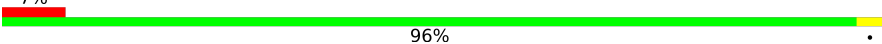
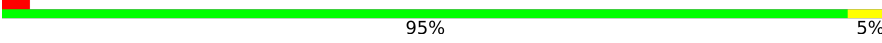
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AAA	234	4% 93% 7%
1	CCC	234	13% 90% 8%
1	EEE	234	14% 90% 8%
1	HHH	234	3% 91% 9%
2	BBB	218	6% 98% .

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Mol	Chain	Length	Quality of chain
2	DDD	218	 5% 97% .
2	FFF	218	 7% 96% .
2	LLL	218	 3% 95% 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14124 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 23ME-00610 Fab (heavy).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	HHH	214	Total	C	N	O	S	4	4	0
			1620	1026	269	319	6			
1	AAA	218	Total	C	N	O	S	3	2	0
			1627	1027	270	324	6			
1	CCC	215	Total	C	N	O	S	6	6	0
			1638	1035	273	324	6			
1	EEE	215	Total	C	N	O	S	4	3	0
			1629	1033	271	319	6			

- Molecule 2 is a protein called 23ME-00610 Fab (light).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	LLL	218	Total	C	N	O	S	6	4	0
			1712	1066	293	347	6			
2	BBB	217	Total	C	N	O	S	3	2	0
			1685	1049	286	345	5			
2	DDD	217	Total	C	N	O	S	13	6	0
			1716	1066	291	354	5			
2	FFF	217	Total	C	N	O	S	6	2	0
			1687	1050	287	345	5			

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

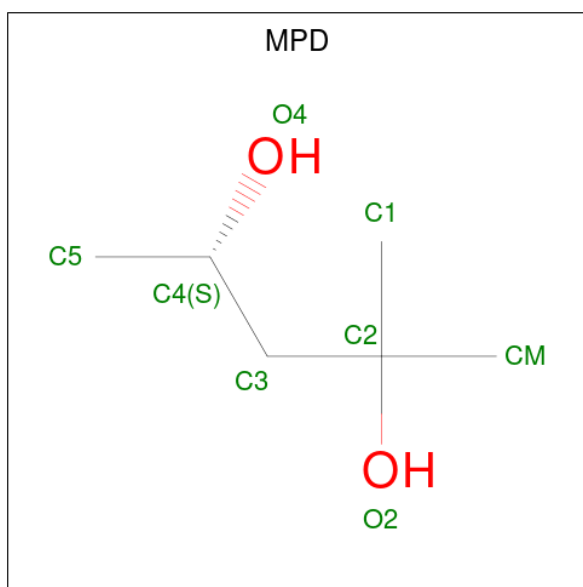
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	HHH	2	Total	Cl	0	0
			2	2		
3	AAA	2	Total	Cl	0	0
			2	2		
3	CCC	2	Total	Cl	0	0
			2	2		
3	EEE	1	Total	Cl	0	0
			1	1		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	HHH	1	Total	O	P	0	0
			5	4	1		
4	AAA	1	Total	O	P	0	0
			5	4	1		
4	CCC	1	Total	O	P	0	0
			5	4	1		
4	CCC	1	Total	O	P	0	0
			5	4	1		
4	EEE	1	Total	O	P	0	0
			5	4	1		
4	EEE	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	HHH	1	Total 8	C 6	O 2	0	0
5	BBB	1	Total 8	C 6	O 2	0	0
5	CCC	1	Total 8	C 6	O 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	HHH	134	Total O 134 134	0	0
6	LLL	123	Total O 123 123	0	0
6	AAA	123	Total O 123 123	0	0
6	BBB	110	Total O 110 110	0	0
6	CCC	64	Total O 64 64	0	0
6	DDD	91	Total O 91 91	0	0
6	EEE	41	Total O 41 41	0	0
6	FFF	63	Total O 63 63	0	0



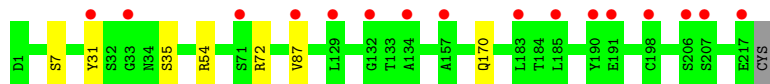
- Molecule 2: 23ME-00610 Fab (light)



- Molecule 2: 23ME-00610 Fab (light)



- Molecule 2: 23ME-00610 Fab (light)



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	225.27Å 67.45Å 136.88Å 90.00° 101.71° 90.00°	Depositor
Resolution (Å)	67.11 – 2.12 67.11 – 2.12	Depositor EDS
% Data completeness (in resolution range)	97.5 (67.11-2.12) 97.5 (67.11-2.12)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.218 , 0.256 0.222 , 0.262	Depositor DCC
R_{free} test set	5592 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14124	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, CL, MPD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AAA	1.03	0/1664	1.28	0/2272
1	CCC	1.05	0/1675	1.30	1/2287 (0.0%)
1	EEE	1.06	0/1668	1.30	0/2278
1	HHH	1.02	0/1657	1.28	0/2262
2	BBB	1.05	0/1721	1.30	1/2337 (0.0%)
2	DDD	1.05	0/1752	1.29	0/2380
2	FFF	1.05	0/1723	1.30	0/2340
2	LLL	1.05	0/1748	1.29	0/2372
All	All	1.04	0/13608	1.29	2/18528 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CCC	111	GLY	CA-C-O	-5.39	118.51	122.23
2	BBB	98	ASP	CA-CB-CG	5.25	117.85	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	1627	0	1616	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CCC	1638	0	1629	1	0
1	EEE	1629	0	1620	3	0
1	HHH	1620	0	1616	2	0
2	BBB	1685	0	1621	1	0
2	DDD	1716	0	1640	1	0
2	FFF	1687	0	1622	3	0
2	LLL	1712	0	1654	6	0
3	AAA	2	0	0	0	0
3	CCC	2	0	0	0	0
3	EEE	1	0	0	1	0
3	HHH	2	0	0	0	0
4	AAA	5	0	0	0	0
4	CCC	10	0	0	0	0
4	EEE	10	0	0	0	0
4	HHH	5	0	0	0	0
5	BBB	8	0	14	0	0
5	CCC	8	0	14	0	0
5	HHH	8	0	14	0	0
6	AAA	123	0	0	0	0
6	BBB	110	0	0	0	0
6	CCC	64	0	0	0	0
6	DDD	91	0	0	0	0
6	EEE	41	0	0	0	0
6	FFF	63	0	0	0	0
6	HHH	134	0	0	1	0
6	LLL	123	0	0	0	0
All	All	14124	0	13060	17	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

The worst 5 of 17 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:LLL:29[A]:VAL:O	2:LLL:29[A]:VAL:HG12	1.92	0.68
2:LLL:29[A]:VAL:O	2:LLL:29[A]:VAL:CG1	2.54	0.55
1:CCC:51:MET:HA	1:CCC:51:MET:HE3	1.91	0.51
2:BBB:87[A]:VAL:HG11	2:BBB:170:GLN:HB3	1.93	0.51
2:FFF:87[A]:VAL:HG11	2:FFF:170:GLN:HB3	1.95	0.49

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	216/234 (92%)	211 (98%)	5 (2%)	0	100	100
1	CCC	217/234 (93%)	212 (98%)	5 (2%)	0	100	100
1	EEE	214/234 (92%)	208 (97%)	6 (3%)	0	100	100
1	HHH	214/234 (92%)	209 (98%)	5 (2%)	0	100	100
2	BBB	217/218 (100%)	212 (98%)	4 (2%)	1 (0%)	24	22
2	DDD	221/218 (101%)	214 (97%)	6 (3%)	1 (0%)	24	22
2	FFF	217/218 (100%)	212 (98%)	4 (2%)	1 (0%)	24	22
2	LLL	220/218 (101%)	213 (97%)	5 (2%)	2 (1%)	14	10
All	All	1736/1808 (96%)	1691 (97%)	40 (2%)	5 (0%)	43	36

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	LLL	72[A]	ARG
2	LLL	72[B]	ARG
2	BBB	72	ARG
2	FFF	72	ARG
2	DDD	72	ARG

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	188/202 (93%)	188 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CCC	189/202 (94%)	186 (98%)	3 (2%)	55	63
1	EEE	187/202 (93%)	187 (100%)	0	100	100
1	HHH	187/202 (93%)	187 (100%)	0	100	100
2	BBB	193/192 (100%)	193 (100%)	0	100	100
2	DDD	197/192 (103%)	195 (99%)	2 (1%)	68	76
2	FFF	193/192 (100%)	192 (100%)	1 (0%)	81	87
2	LLL	196/192 (102%)	194 (99%)	2 (1%)	68	76
All	All	1530/1576 (97%)	1522 (100%)	8 (0%)	81	87

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	FFF	7	SER
2	DDD	131	SER
1	CCC	85[B]	VAL
1	CCC	85[A]	VAL
2	DDD	7	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 7 are monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	PO4	AAA	302	-	4,4,4	0.75	0	6,6,6	0.46	0
5	MPD	BBB	301	-	7,7,7	0.22	0	9,10,10	0.44	0
4	PO4	EEE	302	-	4,4,4	0.67	0	6,6,6	0.49	0
4	PO4	CCC	302	-	4,4,4	0.68	0	6,6,6	0.48	0
4	PO4	CCC	304	-	4,4,4	0.79	0	6,6,6	0.45	0
5	MPD	CCC	303	-	7,7,7	0.17	0	9,10,10	0.37	0
5	MPD	HHH	303	-	7,7,7	0.22	0	9,10,10	0.47	0
4	PO4	HHH	302	-	4,4,4	0.71	0	6,6,6	0.46	0
4	PO4	EEE	303	-	4,4,4	0.68	0	6,6,6	0.48	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MPD	HHH	303	-	-	1/5/5/5	-
5	MPD	BBB	301	-	-	0/5/5/5	-
5	MPD	CCC	303	-	-	0/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	HHH	303	MPD	C2-C3-C4-C5

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	218/234 (93%)	0.45	9 (4%) 41 44	16, 37, 62, 90	4 (1%)
1	CCC	215/234 (91%)	0.99	30 (13%) 6 7	20, 46, 84, 94	9 (4%)
1	EEE	215/234 (91%)	1.17	33 (15%) 5 5	22, 56, 99, 121	5 (2%)
1	HHH	214/234 (91%)	0.37	8 (3%) 45 48	13, 35, 73, 90	5 (2%)
2	BBB	217/218 (99%)	0.64	13 (5%) 27 30	17, 42, 64, 110	5 (2%)
2	DDD	217/218 (99%)	0.66	10 (4%) 37 40	19, 44, 61, 88	15 (6%)
2	FFF	217/218 (99%)	0.78	16 (7%) 20 22	18, 50, 74, 106	7 (3%)
2	LLL	218/218 (100%)	0.58	7 (3%) 50 53	14, 39, 58, 109	9 (4%)
All	All	1731/1808 (95%)	0.71	126 (7%) 21 23	13, 44, 76, 121	59 (3%)

The worst 5 of 126 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	135	SER	5.9
1	EEE	206[A]	LYS	4.3
1	CCC	29	LEU	4.2
1	CCC	31	ASN	3.9
2	LLL	158	LEU	3.7

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MPD	CCC	303	8/8	0.69	0.26	99,102,103,104	0
4	PO4	EEE	303	5/5	0.71	0.15	105,110,112,115	0
5	MPD	BBB	301	8/8	0.72	0.31	82,87,88,90	0
4	PO4	HHH	302	5/5	0.79	0.16	89,93,94,99	0
4	PO4	EEE	302	5/5	0.80	0.13	98,101,104,104	0
4	PO4	CCC	302	5/5	0.80	0.14	108,108,111,113	0
4	PO4	CCC	304	5/5	0.84	0.11	88,89,93,98	0
3	CL	CCC	305	1/1	0.85	0.20	75,75,75,75	0
4	PO4	AAA	302	5/5	0.85	0.14	88,89,89,91	0
5	MPD	HHH	303	8/8	0.87	0.19	62,68,69,71	0
3	CL	EEE	301	1/1	0.90	0.12	60,60,60,60	0
3	CL	CCC	301	1/1	0.93	0.10	54,54,54,54	0
3	CL	HHH	304	1/1	0.96	0.08	55,55,55,55	0
3	CL	HHH	301	1/1	0.98	0.07	39,39,39,39	0
3	CL	AAA	301	1/1	0.98	0.07	41,41,41,41	0
3	CL	AAA	303	1/1	0.98	0.07	43,43,43,43	0

6.5 Other polymers

There are no such residues in this entry.